

On Hidden States in Quantum Random Walks

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Abstract. It was recently pointed out that identifiability of quantum random walks and hidden Markov processes underlie the same principles. This analogy immediately raises questions on the existence of hidden states also in quantum random walks and their relationship with earlier debates on hidden states in quantum mechanics. The overarching insight was that not only hidden Markov processes, but also quantum random walks are finitary processes. Since finitary processes enjoy nice asymptotic properties, this also encourages to further investigate the asymptotic properties of quantum random walks. Here, answers to all these questions are given. Quantum random walks, hidden Markov processes and finitary processes are put into a unifying model context. In this context, quantum random walks are seen to not only enjoy nice ergodic properties in general, but also intuitive quantum-style asymptotic properties. It is also pointed out how hidden states arising from our framework relate to hidden states in earlier, prominent treatments on topics such as the EPR paradoxon or Bell's inequalities.

Keywords. Bell's inequality, EPR paradox, hidden state, Markovian operator, negative probability, quantum Markov chain, quantum measurement

1 Introduction

Quantum random walks were introduced in 2001 [1], as a concept that can emulate Markov chain based techniques on quantum computers [20]. This analogy in terms of application immediately raises questions relating to theoretical analogies. Do quantum random walks have nice asymptotic properties, such as favorable convergence rates? And, when relating quantum random walks to Markovian latent variable models such as hidden Markov processes: are there any reasonable latent variables also in quantum random walks? And, if so, can one perform convenient computations on those hidden states?

Recent research [11] pointed out that both hidden Markov processes and quantum random walks are *finitary*. Finitary processes have been key to determining the equivalence of two differently parametrized hidden Markov processes and, as became clear

in [11], also of two quantum random walks. As was pointed out in [25], finitary processes are also key to determining ergodicity of those processes, in polynomial time with respect to the input parameters. These issues are closely related with the identifiability problem one commonly encounters in latent variable modeling [6,7,17,18]. So these findings put quantum random walks immediately into the focus of questions concerning hidden variables.

Finitary processes can be viewed as acting on underlying hidden states that have been decoupled from probability theory—while hidden states still exist, there is no probabilistic prescription for how they operate [17,10]. While this renders it impossible to estimate in which of those hidden states the system is actually in, this comes with non-negligible benefits in compensation. As above-mentioned, one creates a frame that allows for determining equivalence and ergodicity. Moreover, it allows for (sometimes dramatic) reductions in terms of model complexity. There are examples of stochastic processes, quite intuitively based on only few underlying hidden states, that require an infinite number of hidden states when stipulating probabilistic interpretation in addition (the “probability clock”; see [19]). However, they indeed are based on just the intuitive, finite number of hidden states, if one gets rid of these probabilistic constraints.

The purpose of this paper is to thoroughly explore these relationships. We provide a formal frame that puts hidden Markov processes, quantum random walks and finitary processes into one, unifying context. This frame allows us to prove convenient, quantum-style ergodic properties (“*stationary limit densities*”) for quantum random walks first of all. As a sound justification of our doing, our framework allows us to point out a natural (and, as we feel, quite striking) analogy between finitary processes on the one hand, and the corresponding counterpart emerging from quantum random walks on the other hand. In short, we demonstrate that freeing hidden states from probability theory in the context of stochastic process theory is equivalent to freeing hidden states from being measurable in the context of quantum mechanical counterparts of finitary processes, as a generalization of quantum random walks.

We finally point out that our framework can also draw a connection to (historically prominent) debates on the existence of hidden states within the frame of the quantum mechanics formalism. Examples and results raised around those debates—the EPR paradox and Bell’s inequalities, for example [4,5,8,21,22,24]—can be conveniently rephrased using our framework, which allows to maintain a clear, formal view on possible hidden states in this context.

2 Preliminaries

2.1 Hermitian Matrices

\mathbb{R} denotes the scalar field of real numbers and \mathbb{C} the field of complex numbers $z = a + ib$ (where $a, b \in \mathbb{R}$ and $i^2 = -1$). $\mathbb{C}^{m \times n}$ is the (mn) -dimensional vector space of all $(m \times n)$ -matrices of the form

$$C = A + iB \quad \text{with } A, B \in \mathbb{R}^{m \times n}. \quad (1)$$

$\overline{C} = A - iB$ is the *conjugate* of $C = A + iB$. The transpose $C^* = \overline{C}'$ of its conjugate \overline{C} is the *adjoint* of C . $\mathbb{C}^{m \times n}$ is a Hilbert space with respect to the *Hermitian inner product*

$$\langle C | D \rangle := \text{tr}(C^* D) = \sum_{i=1}^m \sum_{j=1}^n \overline{c_{ji}} d_{ij}, \quad (2)$$

where the c_{ij} and the d_{ij} denote the coefficients of C and D . $\|C\| := \sqrt{\langle C | C \rangle}$ is the *norm* of C . \mathbb{C}^n is short for $\mathbb{C}^{n \times 1}$ and can also be identified with the space of diagonal matrices in $\mathbb{C}^{n \times n}$:

$$\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} \in \mathbb{C}^n \quad \longleftrightarrow \quad \text{diag}(u_1, u_2, \dots, u_n) = \begin{bmatrix} u_1 & 0 & 0 & \dots \\ 0 & u_2 & 0 & \dots \\ \vdots & & \ddots & \\ 0 & \dots & u_n \end{bmatrix} \quad (3)$$

Assuming $m = n$, a matrix $C = A + iB$ with the property $C^* = C$ is *self-adjoint* or *Hermitian*, which means that A is *symmetric* (i.e., $A^T = A$) and B *skew-symmetric* (i.e., $B^T = -B$). Let \mathcal{H}_n denote the collection of all Hermitian ($n \times n$)-matrices. From the general form (1) one recognizes \mathcal{H}_n as a real Hilbert space of dimension $\dim_{\mathbb{R}}(\mathcal{H}_n) = n^2$.

A matrix $Q = [q_{ij}] \in \mathcal{H}_n$ has real eigenvalues λ_i and a corresponding orthonormal set $\{u_1, \dots, u_n\}$ of eigenvectors $u_i \in \mathbb{C}^n$, yielding the *spectral decomposition*

$$Q = \sum_{i=1}^n \lambda_i u_i u_i^* \quad \text{and hence trace} \quad \text{tr}(Q) = \sum_{i=1}^n q_{ii} = \sum_{i=1}^n \lambda_i. \quad (4)$$

$Q \in \mathcal{H}_n$ is said to be *nonnegative* if all eigenvalues of Q are nonnegative, which is equivalent to the property

$$u^* Q u \geq 0 \quad \text{holds for all } u \in \mathbb{C}^n. \quad (5)$$

A vector $u \in \mathbb{C}^n$ gives rise to a nonnegative element $uu^* \in \mathcal{H}_n$ and one has

$$\langle u | u \rangle = \text{tr}(uu^*). \quad (6)$$

In the case $\text{tr}(uu^*) = 1$, the matrix uu^* is thought to represent a *pure state* of an n -dimensional quantum system.

2.2 Unitary Operators

A matrix $U \in \mathbb{C}^{n \times n}$ is *unitary* if the identity matrix I factors into $I = UU^*$, i.e., if the row (or column) vectors of U form an orthonormal basis for \mathbb{C}^n . So also U^* is unitary. For example, an orthonormal basis $\{u_1, \dots, u_n\}$ of eigenvectors relative to $Q \in \mathcal{H}_n$ gives rise to a unitary matrix U^* with columns u_i . Where $\lambda_1, \dots, \lambda_n$ are the corresponding eigenvalues, the linear operator $x \mapsto Qx$ on \mathbb{C}^n is described with respect to the basis U^* via the transformed matrix

$$UQU^* = \text{diag}(\lambda_1, \dots, \lambda_n) \in \mathcal{H}_n. \quad (7)$$

2.3 Strings and Process Functions.

Let Σ be a finite alphabet. We write $a, b \in \Sigma$ for single letters and $v, w \in \Sigma^* = \cup_{t \geq 0} \Sigma^t$ for strings, where $\Sigma^0 = \{\epsilon\}$ with ϵ the *empty string*. Concatenation of $v = v_1 \dots v_t \in \Sigma^t$, $w = w_1 \dots w_s \in \Sigma^s$ is written $vw = v_1 \dots v_t w_1 \dots w_s \in \Sigma^{t+s}$. We consider stochastic processes (X_t) taking values in Σ as string functions $p : \Sigma^* \rightarrow \mathbb{R}$ where

1. $p(v) \geq 0$ for all $v \in \Sigma^*$,
2. $\sum_{a \in \Sigma} p(va) = p(v)$ for all $v \in \Sigma^*$,
3. $p(\epsilon) = 1$.

Such string functions are in one-to-one correspondence with stochastic processes via the relationship [for technical convenience, stochastic processes start at $t = 1$]

$$\mathbf{P}(\{X_1 = v_1, \dots, X_t = v_t\}) = p(v_1 \dots v_t) \quad (8)$$

due to standard measure-theoretic arguments. We refer to such string functions p as *process functions*.

3 Processes

In the following, we will identify *quantum random walks (QRWs)* with the stochastic processes associated with it and we will refer to their parametrizations as QRW parametrizations. Furthermore, we will distinguish between *hidden Markov processes (HMPs)* and *hidden Markov models (HMMs)*, where the latter are the parametrizations of HMPs.

We summarize these facts for introductory purposes only; none of what follows in this section is new. See the citations listed in the following for more details.

3.1 Finitary Processes

As was pointed out in [11], both *hidden Markov processes (HMPs)* and *quantum random walks (QRWs)* are *finitary processes*. While this was new for QRWs, this was well known for HMPs. Finitary processes emerged in early work on HMP identification (e.g. [6,7,14,17]) and have remained a core concept also in recent work on identifiability [13,18,27,29]. Finitary processes are sometimes also referred to as *linearly dependent* [18], *observable operator models* [19] or as *finite-dimensional* [10,25]. In their possibly most prevalent application they served to determine equivalence of hidden Markov processes (HMPs) in 1992 [18]. The exponential runtime algorithm was later improved to polynomial runtime [11].

Definition 1 (Finitary Process) *A stochastic process $p : \Sigma^* \rightarrow \mathbb{R}$ is said to be finitary iff there are matrices $M_a \in \mathbb{R}^{d \times d}$ for all $a \in \Sigma$ and a vector $\pi \in \mathbb{R}^d$ where $[\cdot]^T$ denote matrix transposition and $\mathbf{1}$ be the vector of all ones]*

1. $M := \sum_a M_a$ has unit row sums, i.e. $M\mathbf{1} = \mathbf{1}$ and
2. π is a unit vector, i.e. $\pi^T \mathbf{1} = 1$

such that

$$p(v_1 \dots v_t) = \pi^T M_{v_1} \cdot \dots \cdot M_{v_t} \mathbf{1} \quad (9)$$

Because of $\pi \in \mathbb{R}^d$ and $M_a \in \mathbb{R}^{d \times d}$ for all $a \in \Sigma$, the parametrization $((M_a)_{a \in \Sigma}, \pi)$ is referred to as d -dimensional.

It is an immediate observation that a finitary process that admits a d -dimensional parametrization also admits a parametrization of dimension $d + 1$, which allows for the following definition.

Definition 2 (Rank of a Finitary Process) *The rank of a finitary process (X_t) is the minimal dimension of a parametrization that it admits.*

3.2 Hidden Markov Processes

A hidden Markov process (HMP) is parametrized by a tuple $\mathcal{M} = (S, E, \pi, M)$ where

1. $S = \{s_1, \dots, s_n\}$ is a finite set of “hidden” states
2. $E = [e_{ia}] \in \mathbb{R}^{S \times \Sigma}$ is a non-negative emission probability matrix with unit row sums $\sum_{a \in \Sigma} e_{ia} = 1$, (i.e. the row vectors of E are probability distributions on Σ)
3. π is an initial probability distribution on S and
4. $M = [m_{ij}] \in \mathbb{R}^{S \times S}$ is a non-negative transition probability matrix with unit row sums $\sum_{j=1}^n m_{ij} = 1$ (i.e. the row vectors of M are probability distributions on S)

The associated process (X_t) initially moves to a state $s_i \in S$ with probability $\pi_i := \pi_{s_i}$ and emits the symbol $X_1 = a$ with probability e_{ia} . Then it moves from s_i to a state s_j with probability m_{ij} and emits the symbol $X_2 = a'$ with probability $e_{ja'}$ and so on. In the following, we also refer to a parametrization $\mathcal{M} = (S, E, \pi, M)$ as a *hidden Markov model (HMM)*. See [9] for a comprehensive review.

Remark 1 Replacing the emission probability matrix E by a function $f : S \rightarrow \Sigma$, which models that from hidden state s the value $f(s)$ is observed with probability one, gives rise to a class of processes referred to as finite functions of Markov chains (FFMCs). It is relatively straightforward to observe (see [18]) that the class of hidden Markov processes is equivalent to that of FFMCs.

HMPs are finitary HMPs $p : \Sigma^* \rightarrow \mathbb{R}$ are immediately shown to be finitary by the observation that the transition matrix $M \in \mathbb{R}^{S \times S}$ decomposes as

$$M = \sum_{a \in \Sigma} M_a, \quad \text{with coefficients } (M_a)_{ij} := e_{ia} \cdot m_{ij}. \quad (10)$$

These coefficients reflect the probabilities to emit symbol a from state s_i and to move on to state s_j . Standard technical computations then indeed yield that

$$p(v_1 \dots v_t) = \pi^T M_{v_1} \cdot \dots \cdot M_{v_{t-1}} M_{v_t} \mathbf{1}. \quad (11)$$

This shows p to be a finitary process of rank at most $|S|$, the number of hidden states.

Remark 1 HMPs on d hidden states of rank d and finitary processes that do not admit a HMM parametrization are known to exist. See, for example, Ex. 3.8 in [27] for the former and see [19] for the latter, where the “probability clock” has rank 3 as finitary process, but only admits a HMP formulation on an infinite number of hidden states.

3.3 Quantum Random Walks

In earlier work of ours [11], we had pointed out a connection between *quantum random walks* (QRWs) and finitary processes. We will briefly revisit this connection here for the sake of illustration. In the following, we consider a QRW as given by a unitary operator U together with an initial wave function ψ_0 . Usually, as per a most general definition, the QRW (U, ψ_0) is supposed to reflect the locality structure of P , the probability matrix of a discrete-time Markov chain [28].

Szegedy’s Model. Note that the following example connects finitary processes with a quantum walk model that was raised in a seminal paper [1]. In the meantime, several reformulations of QRWs have been raised, including the popular and attractive one by Szegedy [28]. We note already here that also Szegedy’s model is covered by our treatment. However, while this connection is even easier to draw than for Aharonov et al.’s model [1], it requires to raise the definition of *Quantum Markov Chains* first. See subsection 4.4 for the corresponding arguments.

Aharonov’s Early Model. In the seminal work of [1] (see also [20]), a *quantum random walk* (QRW) is parametrized by a tuple $\mathcal{Q} = (G, U, \psi_0)$ where

1. $G = (\Sigma, E)$ is a directed graph over the alphabet Σ
2. $U : \mathbb{C}^k \rightarrow \mathbb{C}^k$ is a unitary *evolution* operator where $k := |E| = K \cdot |\Sigma|$ and
3. $\psi_0 \in \mathbb{C}^k$ is a wave function, i.e. $\|\psi_0\| = 1$ [$\|\cdot\|$ is the Euclidean norm].

Edges are labeled by tuples (a, x) , $a \in \Sigma$, $x \in X$ where X is a finite set with $|X| = K$. Correspondingly, \mathbb{C}^k is considered to be spanned by the orthonormal basis

$$\langle \mathbf{e}_{(a,x)} \mid (a,x) \in E \rangle.$$

Following the definition of a *general quantum walk* suggested by [1], the unitary operator U is supposed to respect the structure of the graph. That is, if $\mathcal{N}(a) := \{a' \in \Sigma \mid \exists (a, a') \in E\}$ are the neighboring nodes of a , so

$$U(\mathbf{e}_{(a,x)}) \subset \text{span}\{\mathbf{e}_{(a',x)} \mid a' \in \mathcal{N}(a) \cup \{a\}\}.$$

The *quantum random walk* (X_t) arising from a parametrization $\mathcal{Q} = (G, U, \psi_0)$ proceeds by first applying the unitary operator U to ψ_0 and subsequently, with probability $\sum_{x \in X} |(U\psi_0)_{(a,x)}|^2$, “collapsing” (i.e. projecting and renormalizing, which models a quantum mechanical measurement) $U\psi_0$ to the subspace spanned by the vectors $\mathbf{e}_{(a,x), x \in X}$ to generate the first symbol $X_1 = a$. Collapsing $U\psi_0$ results in a new wave function ψ_1 . Applying U to ψ_1 and collapsing it, with probability $\sum_{x \in X} |(U\psi_1)_{(a',x)}|^2$, to the subspace spanned by $\mathbf{e}_{(a',x), x \in X}$ generates the next symbol $X_2 = a'$. Iterative application of U and subsequent collapsing generates further symbols.

Quantum random walks are finitary. Exposing QRWs as finitary, as per the arguments raised in [11], is based on a fundamental theorem for finitary processes.

Definition 3 (Hankel matrix) *Let*

$$\mathcal{P}_p := [p(vw)_{v,w \in \Sigma^*}] \in \mathbb{C}^{\Sigma^* \times \Sigma^*} \quad (12)$$

be the Hankel matrix of a process function $p : \Sigma^ \rightarrow \mathbb{R}$.*

Note that both rows and columns of \mathcal{P}_p

$$p_v : w \mapsto p(vw) \quad \text{and} \quad p^w : v \mapsto p(vw)$$

are string functions in their own right. Note further that $\frac{1}{p(v)}p_v$ is a process function for $p(v) > 0$, while this is not necessarily the case for columns p^w . We refer to row and column space of \mathcal{P}_p as

$$\mathcal{R}(p) = \text{span}\{p_v \mid v \in \Sigma^*\} \quad \text{and} \quad \mathcal{C}(p) = \text{span}\{p^w \mid w \in \Sigma^*\}$$

respectively. Note that, in comparison to earlier work ([11]), we have exchanged rows and columns, for the sake of a more convenient notation.

One can show that finitary processes are precisely the processes whose Hankel matrices have finite rank. In fact, the rank of \mathcal{P}_p is just the rank of p as a finitary process.

Theorem 1 ([19,27]) *Let $p : \Sigma^* \rightarrow \mathbb{C}$ be a process function. Then the following conditions are equivalent.*

- (i) \mathcal{P}_p has rank at most d .
- (ii) *There exists a vector $\pi \in \mathbb{C}^d$ and matrices $M_a \in \mathbb{R}^{d \times d}$ for all $a \in \Sigma$ such that*

$$p(a_1 \dots a_n) = \pi^T M_{a_1} \cdot \dots \cdot M_{a_n} \mathbf{1} \quad (13)$$

for all $v = a_1 \dots a_n \in \Sigma^$.*

The arguments put forward in [11] proceeded further by showing that QRWs $p : \Sigma^* \rightarrow \mathbb{R}$ allow for choosing a finite number of string functions q_1, \dots, q_{k^2} , where k is the number of edges of the graph that underlies the QRW p , such that

$$\mathcal{R}(p) = \text{span}\{q_i \mid i = 1, \dots, k^2\}. \quad (14)$$

That is, the q_i span the row space of \mathcal{P}_p , the Hankel matrix of the QRW p , which exposes p as a finitary process of rank at most k^2 .

4 Quantum Markov Chains

We have just seen (section 3.3) that QRWs are finitary [11]. As a consequence, QRWs come with some convenient properties that have been raised for this class of processes [10,11,25,26].

Convergence rates are a critical issue for QRWs, because QRWs are supposed to emulate Markov Chain Monte Carlo (MCMC) based techniques on quantum computers. This explains why in [1] it was pointed out that the limits

$$\bar{p}(v) := \lim_{t \rightarrow \infty} \sum_{\bar{w} \in \Sigma^t} p(\bar{w}v) \quad (15)$$

for p a QRW (as process function), and v a single letter (node), exist. This justifies QRWs as a reasonable quantum computational concept.

Finitary processes were shown to be *asymptotically mean stationary (AMS)*, see [10]. Therefore, they have good ergodic properties (see [16,15]). An immediate consequence of this is, for example, that one can replace single letters v by arbitrary cylinder sets of strings in (15). Also, the conditional entropies of AMS processes were shown to converge to a limit

$$H_\infty(X) = \lim_{t \rightarrow \infty} \frac{1}{t} H(X^t) = \lim_{t \rightarrow \infty} H(X^t | X^{t-1}) \quad (16)$$

see [16]. In summary, this already significantly generalizes (15).

However, we have not shown limits to exist that have meaning in terms of the QM formalism, and not only in terms of the statistics derived from QRWs. As an illustration for the inherent difficulties, let (U, ψ_0) be a QRW where U does not have 1 as eigenvalue, which implies

$$\lim_{t \rightarrow \infty} \frac{1}{t} \sum_{k=0}^{t-1} U^k \psi_0 = 0. \quad (17)$$

Our wishful thinking, however, was to obtain non-trivial *wave functions* $\bar{\psi}$ as limits. While this is not possible, we will be able to prove the existence of other, truly QM formalism related, meaningful limits later in this treatment.

When generalizing the concept of QRWs in the following, we are aiming at the following two goals:

1. We would like to allow for limits that, unlike (17), also have meaning in terms of QM-related descriptions of systems, beyond the limits so far obtained that have meaning in terms of probability theory (whereof the *stationary limit distributions* of (15) were a special example, and the insight that QRWs are AMS added more of that kind, as pointed out above).
2. We would like to be able to interpret the possible existence of hidden states in these systems in the light of the QM formalism and thereby connect to earlier (well-known and largely inspiring) debates on the existence of hidden states within the QM formalism.

In this section, we make the first step towards such a unifying clarification. We give the definition of a *quantum Markov chain (QMC)* as a generalization of a QRW.

4.1 Definition

In the following, we write

$$\mathcal{V}^+ := \{Q \in \mathcal{V} \mid u^* Q u \geq 0 \text{ for all } u \in \mathbb{C}^n\} \quad (18)$$

for the non-negative elements of $\mathcal{V} \subset \mathcal{H}_n$.

Definition 1 (Quantum Markov Chain). Let $\mathcal{V} \subset \mathcal{H}_k$, $Q_0 \in \mathcal{V}$, Σ be a finite set, and $\mu_a : \mathcal{V} \rightarrow \mathcal{V}$, $a \in \Sigma$ be \mathbb{R} -linear operators. Let $\mu := \sum_a \mu_a$. We refer to the tuple

$$(\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q_0) \quad (19)$$

as quantum Markov chain iff

$$Q_0 \in \mathcal{V}^+ \quad (20)$$

$$\text{tr } Q_0 = 1 \quad (21)$$

$$\text{for all } Q \in \mathcal{V} : \text{tr } \mu(Q) = \text{tr } Q \quad (22)$$

$$\text{for all } a \in \Sigma : \mu_a(\mathcal{V}^+) \subset \mathcal{V}^+ \quad (23)$$

REMARK.

- If the μ_a are *completely positive*, that is

$$(I \otimes \mu_a)(A) \geq 0 \quad \text{for any nonnegative } A \in \mathcal{W} \otimes \mathcal{V} \quad (24)$$

where \mathcal{W} is an extra system, the μ_a are *quantum operations* (cf. [23]). The quantum operations formalism aims at modeling the dynamics of open quantum systems and quantum noise, borrowing from the interrelation between classical noise and classical Markov chains. Time-discrete quantum Markovian dynamics have also been described by trace-preserving quantum operations as *quantum channels* (see, e.g., [30]).

- If the μ_a reflect quantum operations, as described above, then the collection

$$\{\mu_a \mid a \in \Sigma\} \quad (25)$$

is also referred to as *measurement model* in the literature, see [23].

- So, when requiring the μ_a to be completely positive, the QMCs provide a means for extending those formalisms towards a clearer view on their (potential) hidden states and their temporal dynamics, hence their asymptotic, ergodic properties. While we could be happy to postulate complete positivity—which would not interfere with any of the following theoretical results—we refrain from explicitly doing so, for the sake of a clearer technical exposition.

Let $\mu_v := \mu_{v_t} \dots \mu_{v_1}$ for $v = v_1 \dots v_t$ [note the reverse order on the letters]. Quantum Markov chains can be seen to give rise to stochastic processes p (viewed as process functions, see section 2.3) by the rule

$$p(v) := \text{tr } \mu_v(Q_0) \quad (26)$$

The defining properties immediately imply that

$$\text{tr } \mu_v Q_0 \in [0, 1] \quad \text{for all } v \in \Sigma^* \quad (27)$$

since [the first equation will follow from multinomial expansion]

$$\sum_{v \in \Sigma^t} \text{tr } \mu_v Q_0 = \text{tr } \mu^t Q_0 \stackrel{(22)}{=} \text{tr } Q_0 \stackrel{(21)}{=} 1. \quad (28)$$

This, by further means of (20,23) shows that

$$[\text{tr } \mu_v Q_0]_{v \in \Sigma^t} \quad (29)$$

establishes a probability distribution over Σ^t . We recall (1),(2),(3) of section 2.3 to see that p corresponds to a stochastic process.

We list some relationships of the elements of quantum Markov chains with existing concepts of Markov chain theory and quantum mechanics in the following subsections.

4.2 Unitary Evolution

In quantum mechanics, evolution is described by application of unitary matrices $U \in \mathbb{C}^{n \times n}$ to wave functions $\phi \in \mathbb{C}^n$ (that is $\|\phi\| = 1$), which results in a new wave function $U\phi$ where $\|U\phi\| = 1$ since U is unitary. In terms of densities $Q = \psi\psi^*$, this translates into the computation

$$Q \mapsto UQU^* \quad (30)$$

which establishes a linear, non-negative and trace-preserving operation $\mu_U : \mathcal{H}_n \rightarrow \mathcal{H}_n$. Time-discrete, unitary evolution can therefore be modeled in form of QMCs

$$(\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q_0) \quad \text{where} \quad |\Sigma| = 1 \quad (31)$$

such that

$$\mu = \mu_a : \mathcal{V} \rightarrow \mathcal{V}, Q \mapsto UQU^* \quad (32)$$

with unitary U describing evolution of the system.

4.3 Measurements

A (positive operator valued) quantum measurement (= POVM, cf. [3,23]) is given by a finite collection $X = \{M_a \mid a \in \Sigma\}$ of matrices $M_a \in \mathbb{C}^{n \times n}$ such that the self-adjoint matrices $X_a = M_a M_a^*$ are non-negative and sum up to the identity:

$$I = \sum_{a \in \Sigma} X_a = \sum_{a \in \Sigma} M_a M_a^*. \quad (33)$$

POVMs give rise to QMCs by raising linear operators

$$\mu_a : \mathcal{H}_n \rightarrow \mathcal{H}_n, Q \mapsto M_a Q M_a^* \quad (34)$$

together with a quantum density Q_0 . Approving the defining principles of QMCs then is an easy exercise.

4.4 Quantum Random Walks

Aharonov et al.'s Model. QRWs $\mathcal{Q} = (G, U, \psi_0)$ are seen to be QMCs, by first introducing projection operators [we remind that $k = |X| \cdot |\Sigma|$ is the number of edges of the walk]

$$P_a : \mathbb{C}^k \longrightarrow \mathbb{C}^k, \psi \mapsto \sum_{(a,x), x \in X} \psi_{(a,x)} \mathbf{e}_{(a,x)}$$

which project vectors onto the subspace spanned by basis vectors (which are in a one-to-one correspondence with the edges) associated with the letter a , and further setting

1. $\mathcal{V} := \mathcal{H}_k$
2. $Q_0 := \psi_0 \psi_0^* \in \mathbb{C}^{k \times k}$
3. $\mu_a : \mathcal{H}_k \longrightarrow \mathcal{H}_k, Q \mapsto (P_a U) Q (P_a U)^*$.

Szegedy's Model. According to Szegedy [28], the unitary operator U is supposed to agree with a unitary operator $W_{P,Q}$, where the probabilistic matrices P, Q give rise to a *bipartite random walk*. So, identifying U in a QRW with some $W_{P,Q}$ in a QRW (U, ψ_0) yields a QRW in the style of Szegedy. This then further translates into identifying also Szegedy-style QRWs with QMCs.

In Szegedy's model, just as in all more advanced QRW models, realizing trajectories of observables is not necessarily in the focus. Rather, letting U evolve for some time t (which results in $U^t \psi_0$), and making predictions about the expected behavior when trying to realize an observable after time t is of interest.

Such studies are, of course, equally covered by our treatment. In particular, we have just pointed out that unitary evolution in itself can be regarded as a QMC, see subsection 4.2 above. However, when trying to associate genuine stochastic processes with QRWs in a physically natural way, then repeated measurements seem to be the only option.

4.5 Hidden Markov Processes

Moreover, one can model hidden Markov processes as QMCs. Therefore, we consider the space \mathcal{D} of diagonal matrices $D \in \mathcal{H}_n$. Let M be the transition probability matrix of a hidden Markov process. We see that

$$\mu(\text{diag}(\pi)) = \text{diag}(\pi^T M) \quad (\pi \in \mathbb{R}^n), \quad (35)$$

establishes a non-negative, trace-preserving linear operator. Decomposing M into matrices M_a , as per $(M_a)_{ij} = e_{ia} \cdot m_{ij}$ (see (10)), we obtain non-negative linear operators

$$\mu_a : \mathcal{D} \rightarrow \mathcal{D}, \text{diag}(\pi) \mapsto \text{diag}(\pi^T M_a) \quad (36)$$

where, obviously, $\sum_a \mu_a = \mu$. It is easy to see that

$$(\mathcal{D}, (\mu_a)_{a \in \Sigma}, \text{diag}(\pi)) \quad (37)$$

is a QMC whose associated stochastic process is that of the hidden Markov process we started from.

Remark 2 *It is an immediate observation that there are HMPs that are not QRWs and vice versa. This exposes both HMPs and QRWs as proper subclasses of QMCs.*

4.6 Hidden States

Representing HMPs as QMCs leads to a one-to-one correspondence of hidden states with the eigenstates of the quantum density $\text{diag}(\pi)$ of the QMC. In QRWs, the natural idea of hidden states is, in many edge-based formulations (in particular in the early one raised by Aharonov et al. [1] discussed above) that of the edges: while one directly observes (sequences of) nodes, one does not necessarily observe the path of edges that leads to the nodes observed. Note that the definition of a QRW does not necessarily imply a one-to-one correspondence of edge paths with sequences of vertices—multiple edges connecting the same pair of nodes might be possible.

Remark. Note that in Szegedy’s model [28] edges do no longer play an explicit role. Nevertheless, pairs of nodes, and not nodes themselves, correspond to basis vectors of the underlying Hilbert spaces. So, *mutatis mutandis*, our considerations also apply for Szegedy’s model in the following. Pairs of nodes, as a concept that is more general than edges, represent hidden states. Also, it is immediately possible to measure hidden states, which corresponds to projecting to the subspace spanned by just one pair of nodes.

Interestingly, this canonical idea of hidden states in QRWs leads to the same analogy: when turning a QRW (U, ψ_0) into a QMC $(\mathcal{V}, (\mu_v)_{v \in V}, Q)$ as described above, edges (or, more general, pairs of nodes), as canonical basis vectors of the underlying Hilbert space turn out to be in a one-to-one correspondence with eigenstates of the quantum density $Q = \psi_0 \psi_0^*$.

When modeling hidden states as eigenspaces, the natural question that arises is whether one can access the hidden states through QM formalism related operations. The immediate answer is yes. Let $\mathbf{q}_1, \dots, \mathbf{q}_n$ be the (orthonormal) eigenstates of Q . Let $P_i : \mathbb{C}^n \rightarrow \mathbb{C}^n$ be the operators that project vectors onto the eigenspaces. Since the P_i are non-negative, and since

$$I = \sum_i P_i P_i^* \quad (38)$$

the P_i are a POVM.³ Let

$$T_i : \mathcal{H}_n \rightarrow \mathcal{H}_n; \quad Q \mapsto P_i Q P_i^* \quad (39)$$

be the corresponding linear operators acting on the densities. Then

$$p(i) := \text{tr } T_i Q \quad (40)$$

correspond to the probability to measure that the system described by Q is in hidden state i .

It is therefore possible to compute probability distributions on paths of hidden states being taken, and, correspondingly, the most likely path being taken (the *Viterbi path*), just as is possible for HMPs.

³ In fact, in more restrictive, classical QM formalism treatments, projections are the only formal description of quantum measurements.

5 Quantum Predictor Models

QMCs have made a first important step towards the unification of the concepts of QRWs and HMPs. In fact, we have shown that both QRWs and HMPs are (proper) subclasses of QMCs. For the relationships raised in earlier work, which aimed at testing equivalence of processes in particular [11,18], there are some important questions left to be answered.

- How do finitary processes relate with QMCs?
- Can this relationship be expressed in QM formalism compatible terms?

As we will show in the following, these questions can be answered in a satisfying way. In fact, finitary processes seem to be the natural, unifying terminal of this treatment.

In order to provide answers, we first recall a natural interpretation of finitary processes: While (a finite number of) hidden states that underlie the system might still exist, transition of hidden states is decoupled from probability theory. This yields that one can no longer compute most likely hidden states relative to the symbols observed. Indeed, the hidden states only make part of the description of the system—namely, if given a finitary process as per a parametrization $((M_a)_{a \in \Sigma}, \pi)$ where $M_a \in \mathbb{R}^{d \times d}, \pi \in \mathbb{R}^d$, hidden states are in a one-to-one correspondence with the canonical basis vectors of \mathbb{R}^d . $M = \sum_a M_a$ then is a parametric (but not necessarily probabilistic!) description of how they change. In non-HMP finitary processes, hidden states *remain (eternally) hidden* to the outside observer, who is not in possession of their parametric description—the observer even fails to compute reasonable estimates about them.

In exchange, freeing hidden states from probability theory comes with clear practical benefits:

- One can achieve dramatic reductions in terms of model complexity. See, for example, the (also aforementioned) “probability clock” [19]: a finite parametrization is only possible when not requiring transitions of hidden states to be probabilistic.
- This idea was key to providing algorithmic solutions for the *identifiability problem*, see [11,18,27], for example.

We will therefore generalize the concept of QMCs to *quantum predictor models* (QPMs). One can characterize QPMs as QMCs where one is no longer guaranteed that performing measurements on hidden states will work. Still, however, these hidden states are clearly visible entities of the description of the system.

We then show that the stochastic processes associated with QPMs are precisely the finitary ones. This raises the following analogy:

1. The step from HMPs to finitary processes needs one to free hidden states from the laws of probability theory.
2. The step from QRWs to finitary processes needs one to free hidden states from being QM-measurable.

Beyond the demonstration of these analogies, we owe the reader a theorem that QM formalism compatible, stationary limits exist. We will do this in the frame of QPMs as well.

5.1 Definition

Definition 2 (Quantum Predictor Model). Let $\mathcal{V} \subset \mathcal{H}_N$, $Q_0 \in \mathcal{V}$, Σ be a finite set, and $\mu_a : \mathcal{V} \rightarrow \mathcal{V}$, $a \in \Sigma$ be \mathbb{R} -linear operators. Let $\mu := \sum_a \mu_a$ and $\mu_v := \mu_{v_l} \circ \dots \circ \mu_{v_1}$ for $v = v_1 \dots v_l$. We refer to the tuple

$$(\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q_0) \quad (41)$$

as quantum predictor model (QPM) iff

$$\text{tr } Q_0 = 1 \quad (42)$$

$$\text{for all } Q \in \mathcal{V} : \text{tr } \mu(Q) = \text{tr } Q \quad (43)$$

$$\text{for all } v \in \Sigma^* : \text{tr } \mu_v Q_0 \in [0, 1] \quad (44)$$

In analogy to Markov chain theory, we refer to a QPM as stationary iff

$$\mu(Q) = Q. \quad (45)$$

For a better structural grasp, we also give the following definition.

Definition 3. Let $Q \in \mathcal{H}_N$ and $\mu : \mathcal{V} \rightarrow \mathcal{V}$ where $\mathcal{V} \subset \mathcal{H}_N$ is a linear subspace.

- We refer to Q as a generalized density iff $\text{tr } Q = 1$.
- We refer to a trace-preserving linear operator $\mu : \mathcal{V} \rightarrow \mathcal{V}$ as a generalized evolution operator.
- We refer to (μ, Q) as generalized Markov chain iff
 - Q is a generalized density and
 - μ is a generalized evolution operator.

Note immediately that generalized Markov chains contain ordinary Markov chains, as per the arguments raised in section 4.5.

We summarize the relationships of quantum predictor models with our previous terms.

Proposition 1. Let $(\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q_0)$ be a QPM.

1. $(X_t)_{t \geq 1}$, given by $p(v_1 \dots v_t) := \mathbb{P}(\{X_1 = v_1, \dots, X_t = v_t\}) := \text{tr } \mu_v Q_0$ establishes a one-sided stochastic process.
2. (μ, Q_0) is a generalized Markov chain in the sense of definition 3.
3. When the μ_a are non-negative (that is, preserve \mathcal{V}_+) and Q_0 is a quantum density, the QPM is a QMC.

Proof. 1. follows from the fact that the combination of (42),(43),(44) yield that p is a process function, 2. and 3. are trivial consequences of the respective definitions. \diamond

5.2 Quantum Predictor Models and Finitary Processes

Theorem 1. *The class of finitary processes is equivalent to the one associated with quantum predictor models.*

Proof. We first show that processes associated with QPMs are finitary. Let p be the process associated with a QPM $(\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q_0)$ where $\dim \mathcal{V} = d$. We choose a basis (Q_1, \dots, Q_d) of \mathcal{V} and consider the matrix

$$II := (\text{tr } \mu_v Q_i)_{i \in \{1, \dots, d\}, v \in \Sigma^*} \in \mathbb{R}^{d \times \Sigma^*},$$

which, because of the finite number of rows, has finite rank. For all $v \in \Sigma^*$, we set

$$\mu_v Q_0 =: \sum_{i=1}^d \alpha_{i,v} Q_i$$

to realize that

$$p(vw) = \text{tr } \mu_w \mu_v Q_0 = \text{tr } \mu_w \sum_{i=1}^d \alpha_{i,v} Q_i = \sum_{i=1}^d \alpha_{i,v} \text{tr } \mu_w Q_i$$

That is, the rows of \mathcal{P} turn out to be linear combinations of rows of II , which implies that the rank of \mathcal{P} is finite.

For the other direction, let $p(v_1 \dots v_t) := \mathbb{P}(\{X_1 = v_1, \dots, X_t = v_t\})$ be the process function of a finitary process (X_t) . Let $\mathcal{P} := [p(vw)_{v,w \in \Sigma^*}]$ be the corresponding Hankel matrix of finite rank d . Let $p_v := (p(vw)_{w \in \Sigma^*})$ denote a row of \mathcal{P} . Let further

$$\mathcal{V}_p := \text{span}\{p_v \mid v \in \Sigma^*\} \quad (46)$$

denote the *row space* of \mathcal{P} , which is of dimension d .

According to the theory of finitary processes (e.g. [11]), one can choose process functions $p_i : \Sigma^* \rightarrow \mathbb{R}, i = 1, \dots, d$ that span the row space. That is, one can write each row

$$p_v = \sum_i \alpha_{v,i} p_i$$

as a linear combination of the p_i . We further observe that $\tau_a : \mathbb{R}^{\Sigma^*} \rightarrow \mathbb{R}^{\Sigma^*}$, defined by $(\tau_a p)(w) := p(aw)$ establishes a linear operator on the space of real-valued string functions. Since obviously

$$\tau_a p_v = p_{va} \quad (47)$$

τ_a preserves the row space of \mathcal{P} . Building on this, let $\alpha_{aij} \in \mathbb{R}$ be defined through the relationship

$$\tau_a p_i = \sum_{j=1}^d \alpha_{aij} p_j \quad (48)$$

We now set

$$D_i := \text{diag}(0, \dots, 0, \underset{i}{1}, 0, \dots, 0)$$

and let $\mathcal{V} := \text{span}\{D_i, i = 1, \dots, d\}$ be the corresponding subspace of \mathcal{H}_d . We define the linear operators $\mu_a : \mathcal{V} \rightarrow \mathcal{V}$ by

$$\mu_a(D_i) := \sum_{j=1}^d \alpha_{aij} D_j, \quad (49)$$

on the basis $(D_i)_{i=1, \dots, d}$ and further through linear extension to all of \mathcal{V} . Let further the coefficients α_{0i} be given through the relationship [note that $p = \mathcal{P}_\epsilon$ is an element of the row space]

$$p =: \sum_{i=1}^d \alpha_{0i} p_i$$

and set

$$Q_0 := \text{diag}(\alpha_{01}, \dots, \alpha_{0d}).$$

We will show that the tuple $\mathcal{Q}_p := (\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q_0)$ yields a QMP which is equivalent to p .

We note first that the μ_a are linear operators by definition. From

$$\text{tr } Q_0 = \sum_{i=1}^d \alpha_{0i} = \sum_{i=1}^d \alpha_{0i} \underbrace{p_i(\epsilon)}_{=1} = p(\epsilon) = 1$$

we obtain (42). To show (43), we compute for $Q \in \mathcal{V}$ and $\mu = \sum_a \mu_a$

$$\begin{aligned} \text{tr } \mu(Q) &= \text{tr } \sum_{a \in \Sigma} \mu_a(Q) = \sum_{a \in \Sigma} \text{tr } \mu_a(Q) \\ &\stackrel{(*)}{=} \sum_{a \in \Sigma} \sum_{i=1}^d \sum_{j=1}^d \alpha_{aij} Q_{ii} = \sum_{i=1}^d Q_{ii} \sum_{a \in \Sigma} \sum_{j=1}^d \alpha_{aij} \\ &= \sum_{i=1}^d Q_{ii} \sum_{a \in \Sigma} \sum_{j=1}^d \alpha_{aij} p_j(\epsilon) = \sum_{i=1}^d Q_{ii} \sum_{a \in \Sigma} (\tau_a p_i)(\epsilon) \\ &= \sum_{i=1}^d Q_{ii} \sum_{a \in \Sigma} p_i(a) = \sum_{i=1}^d Q_{ii} = \text{tr } Q \end{aligned}$$

where $(*)$ just reflects the linear extension of (49) [note that $Q = \sum_{i=1}^d Q_{ii} D_i$], and the last equation follows from the fact that p_i is associated with a stochastic process, which implies $\sum_a p_i(a) = 1$.

In the following, let $v = v_1 \dots v_t \in \Sigma^t$ and $\tau_v := \tau_{v_t} \circ \dots \circ \tau_{v_1}$. We will show that

$$\text{tr } \mu_v(Q_0) = \text{tr } \mu_{v_t} \circ \dots \circ \mu_{v_1}(Q_0) = p(v) \in [0, 1] \quad (50)$$

which yields (44) and the fact that the QPM emerging from \mathcal{Q}_p is equivalent with p , which completes the proof.

Therefore, for a word $v \in \Sigma$ and a vector $h \in \mathcal{V}_p$ (see (46)), we write

$$\tau_v h = (\tau_v h)_i p_i,$$

that is, the $(\tau_v h)_i$ are the coefficients of the representation of $\tau_v h$ over the basis (p_i) . We then show more generally that

$$(\mu_v Q_0)_{ii} = (\tau_v p)_i, \quad (51)$$

which implies the claim because of

$$\text{tr } \mu_v(Q_0) = \sum_i (\tau_v p)_i = \sum_i (\tau_v)_i p_i(\epsilon) = \tau_v p(\epsilon) = g(v).$$

We finally show (51) by induction over t . For $t = 1$ and $a \in \Sigma$ it holds that (note: $\alpha_{a i j} = (\tau_a p_i)_j$)

$$\begin{aligned} (\mu_a Q_0)_{ii} &= \sum_{j=1}^d \alpha_{a j i} \alpha_{0 j} = \sum_{j=1}^d \alpha_{0 j} (\tau_a p_j)_i \\ &= \sum_{j=1}^d (\tau_a (\alpha_{0 j} p_j))_i = \tau_a \left(\sum_{j=1}^d \alpha_{0 j} p_j \right)_i = (\tau_a p)_i, \end{aligned}$$

which makes the start of the induction. Let now $t \geq 1$ and $v = a_1 \dots a_t a_{t+1} \in \Sigma^{t+1}$. Then it holds that

$$\begin{aligned} (\mu_v Q_0)_{ii} &= (\mu_{a_{t+1}} (\mu_{a_1 \dots a_t} Q_0))_{ii} = \sum_{j=1}^d \alpha_{a_{t+1} j i} (\mu_{a_1 \dots a_t})_{j j} \\ &\stackrel{(IV)}{=} \sum_{j=1}^d \alpha_{a_{t+1} j i} (\tau_{a_1 \dots a_t} p)_j = \sum_{j=1}^d (\tau_{a_{t+1}} (\tau_{a_1 \dots a_t} p)_j p_j)_i \\ &= (\tau_{a_{t+1}} \left(\sum_{j=1}^d (\tau_{a_1 \dots a_t} p)_j p_j \right))_i = (\tau_v p)_i. \end{aligned}$$

◇

5.3 Asymptotic Convergence

In the following we will point out that a special class of QPMs, which contains the class of QMCs hence also QRWs have *stationary limit densities*. So, we provide a theorem that ensures convenient asymptotic ergodic properties for QRWs also in terms of the underlying quantum concepts. This is what we were aiming at—we recall that the attempt to compute *stationary limit wave functions* (see (17)) did not lead to success.

Definition 4. Let $\mathcal{Q} = (\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q)$ be a QPM and $\mu := \sum_{a \in \Sigma} \mu_a$ its evolution operators. We say that \mathcal{Q} is bounded if there is a $c \in \mathbb{R}$ such that

$$\langle \mu^t(Q) | \mu^t(Q) \rangle = \text{tr}(\mu^t(Q)^2) \leq c \quad \text{holds for all } t. \quad (52)$$

Proposition 2. Let $\mathcal{Q} = (\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q)$ be a QMC. Then \mathcal{Q} is bounded.

Proof. $\mu^t(Q)$ is a quantum density and therefore satisfies $\text{tr}(\mu^t(Q)^2) \leq 1$. \diamond

We are able to raise the following theorem for bounded QPMs.

Theorem 2. Let $\mathcal{Q} = (\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q)$ be a bounded QPM with evolution operator $\mu = \sum_a \mu_a$. Then the limit of averages

$$\tilde{Q} = \lim_{t \rightarrow \infty} \frac{1}{t} \sum_{k=1}^t \mu^k(Q) \quad (53)$$

exists. Moreover, $\mathcal{Q} = (\mathcal{V}, (\mu_a)_{a \in \Sigma}, \tilde{Q})$ is stationary and if Q is a quantum density, so is \tilde{Q} .

If the limit (53) exists, it is clear that $\text{tr}(\tilde{Q}) = \text{tr}(Q) = 1$ holds and \mathcal{Q} is stationary. Moreover, if μ preserves quantum densities, then each $\mu^t(Q)$, and therefore each average, is a quantum density. So it remains to prove the existence of \tilde{Q} . It is convenient to base the proof on the following lemma.

Lemma 1 ([10]). Let V be a finite-dimensional normed vector space over \mathbb{C} and consider the linear operator $F : V \rightarrow V$. The following statements are equivalent:

- (a) $\bar{v} = \lim_{t \rightarrow \infty} \frac{1}{t} \sum_{k=1}^{t-1} F^k(v)$ exists for all $v \in V$.
- (b) For every $v \in V$, there exists some finite bound $c^* \in \mathbb{R}$ such that $\|F^t(v)\| \leq c^*$ holds for all $t \geq 0$.

We want to apply Lemma 1 to

$$V := \text{span}\{\mu^t Q \mid t \geq 0\} \quad \text{with the norm} \quad \|C\| = \sqrt{\text{tr}(C^* C)}. \quad (54)$$

To this end, we choose $t_0 = 0, t_1, \dots, t_m$ such that $\{Q_j := \mu^{t_j}(Q)\}$ is a basis for V . Let $F := \mu|_V$ be the restriction of μ on V (note that V may be smaller than \mathcal{V} , while $F(V) \subset V$). That is,

$$F\left(\sum_{j=0}^m r_j Q_j\right) := \sum_{j=0}^m r_j \mu(Q_j). \quad (55)$$

Let c be the bound on \mathcal{Q} . We observe from the triangle inequality:

$$\|F^t\left(\sum_{i=1}^m r_i Q_i\right)\| \leq \sum_{i=1}^m |r_i| \cdot \|\mu^t(Q_i)\| = \sum_{i=1}^m |r_i| \cdot \|\mu^{t+t_j}(Q)\| \leq \sum_{i=1}^m |r_i| \sqrt{c} =: c^*. \quad (56)$$

So F satisfies condition (b) and hence also (a) of Lemma 1, which establishes the convergence of the averages in Theorem 2 with the choice $v = P$. \diamond

Corollary 1. *Let $\mathcal{Q} = (\mathcal{V}, (\mu_a)_{a \in \Sigma}, Q)$ be a bounded QPM and $X : \mathcal{H}_n \rightarrow \mathbb{R}$ any linear functional. Then*

$$\lim_{t \rightarrow \infty} \frac{1}{t} \sum_{k=1}^t X(\mu^k(P)) = X(\tilde{P}). \quad (57)$$

◇

Recalling Corollary 2 and combining it with the insight that QRWs are QMCs, we obtain the following novel insight for quantum random walks.

Corollary 2. *Quantum random walks, in their most general form, have stationary limit densities, hence stationary limit distributions, in the sense of Corollary 1.*

Note that the limit distributions one can derive via corollary 1 substantially generalize the limit distributions (15) raised in [1].

6 Relationship with Hidden States in Quantum Mechanics

Hidden states in quantum mechanics have played a prominent role in the frame of debates on the EPR paradox [8] and Bell's inequalities [4,5]. For a consistent treatment, we will rephrase the issue using our own terms.

Remark. What follows is by no means supposed to be a re-interpretation of physical reality, and in that sense it is not supposed to be *realistic* (in the lay sense of the word). The purpose of this section is to point out an analogy between classical stochastic process theory and the QM formalism. The section will deal with the consequences that one has to take into account when making the step from proper random walk models towards finitary models. It is important to understand that, in classical information theory, finitary processes can be viewed as an attempt to “save” hidden states. The problem is that one can no longer apply probability theory when dealing with the “saved” hidden states. This means a certain price for the flexibility that one gains with finitary processes over (the more rigid) hidden Markov processes.

This section is about the price one has to pay when trying to “save” hidden states (in Einstein's sense) when making the step from the still QM formalism compatible Quantum Markov Chains towards the (no longer QM formatlism compatible) Quantum Predictor Models. Similar to classical theory, the gain in doing this is the added flexibility of Quantum Predictor Models over Quantum Markov Chains when it comes to considering asymptotic behavior of Quantum Random Walk like concepts.

Notation. Let \mathfrak{S} be a physical system and assume that there is a finite set $\Omega = \{\omega_1, \dots, \omega_N\}$ of *hidden states* such that \mathfrak{S} is (definitely) in one of the N possible hidden states $\omega \in \Omega$ at any discrete time $t = 0, 1, \dots$. We refer to a function

$$X : \Omega \rightarrow \Sigma \quad (58)$$

as *information function*. Since Ω is finite, we may assume Σ to be finite as well. Σ is supposed to consist of values that one can observe *via quantum measurements*.

Remark 3 Here and in the following, we could assume that $X(\omega)$ is a probability distribution over Σ , in analogy to the probabilistic relationship between hidden states and emitted values (emission probabilities) in hidden Markov processes. Thereby, we would not generalize any of our arguments. Note that HMPs can also be modeled as functions on finite Markov chains (FFMCs) [18], which model a deterministic relationship between hidden states and observed values in HMPs. Analogous arguments apply in our case (we refrain from making them explicit). For these good reasons, we do not assume a probabilistic relationship here.

Hidden States. While one can observe values from Σ , this may not be possible for the hidden states $\omega \in \Omega$. As usual, \mathfrak{S} is described (at a given time t) by a density Q . Given Q , X can be expressed in terms of a POVM $X = \{M_a \mid a \in \Sigma\}$ where

$$\sum_{a \in \Sigma} M_a M_a^* = I \quad \text{and} \quad \text{tr}(M_a Q M_a^*) \geq 0 \quad (59)$$

This establishes that $\text{tr}(M_a Q M_a^*)$, $a \in \Sigma$ establishes a probability distribution on Σ . We write $p_Q(a)$ for such probabilities.

In analogy to the concept of hidden states raised for QPMs, we associate hidden states with the eigenstates of the (initial, at time $t = 0$) density Q . Let P_ω be the projection onto the eigenspace of the hidden state ω (if we model temporal dynamics, we fix those projections—they always refer to the initial eigenstates). Let q_ω be the eigenvalue of Q relative to the eigenspace of ω . That is,

$$q_\omega = \text{tr} P_\omega Q P_\omega^* \quad (60)$$

where, in case of a non-negative density Q , the q_ω are non-negative and sum up to one, which models that one can measure them. This, however, is not necessarily the case for generalized densities Q , which models that one *cannot measure the hidden states*—there are no apparatuses that allow to do that.

When combining *non-measurable hidden states* with *measurable information functions* X , we can see that the measurement M_a corresponds to a projection onto the subspace spanned by the eigenspaces of ω where $X(\omega) = a$. That is, the probability $p(a) = \text{tr} M_a Q M_a^*$ to observe a on Q can be computed as

$$p_Q(a) = \sum_{\omega: X(\omega)=a} q_\omega = \sum_{\omega: X(\omega)=a} \text{tr} P_\omega Q P_\omega^*. \quad (61)$$

In case of real-valued information functions $X : \Omega \rightarrow \Sigma \subset \mathbb{R}$, this implies that one can compute the well-defined expectation

$$E_Q(X) := \sum_{x \in \Sigma} x \cdot p_Q(x) = \sum_{x \in \Sigma} \sum_{\omega: X(\omega)=x} x \cdot q_\omega. \quad (62)$$

Using this setting, one can model the conflicts encountered in prominent treatments referring to the EPR paradox, such as [12,24], as attempts to jointly perform measurements on information functions $X_1 : \Omega \rightarrow \Sigma_1, \dots, X_k : \Omega \rightarrow \Sigma_k$ such that certain

tuples $(a_1, \dots, a_k) \in \Sigma_1 \times \dots \times \Sigma_k$ lead to identification of hidden states whose eigenvalues are negative.

To make this explicit, we give the following definition.

Definition 4 *We say that the k information functions*

$$(X_i : \Omega \rightarrow \Sigma_i)_{i=1, \dots, k} \quad (63)$$

on the system \mathfrak{S} , reflected by the density Q , are jointly observable relative to Q if the composite information function $X : \Omega \rightarrow \Sigma$ with

$$X(\omega) := (X_1(\omega), \dots, X_k(\omega)) \quad \text{and} \quad \Sigma := \Sigma_1 \times \dots \times \Sigma_k \quad (64)$$

is observable in Q .

If $(X_i : \Omega \rightarrow \Sigma_i)_{i=1, \dots, k}$ are jointly observable relative to Q , so for each $(a_1, \dots, a_k) \in \Sigma_1 \times \dots \times \Sigma_k$ there is $M_{(a_1, \dots, a_k)}$ such that

$$p_Q(a_1, \dots, a_k) := \text{tr } M_{a_1, \dots, a_k} Q M_{a_1, \dots, a_k}^* \quad (65)$$

is the probability to observe (a_1, \dots, a_k) . Note that in our setting

$$M_{a_1, \dots, a_k} = M_{a_1} \cdot \dots \cdot M_{a_k} \quad (66)$$

since each of the measurements M_a reflects a projection on a subspace.

Remark 4 *This precisely is the benefit of our setting—it allows to have a clear formal view on hidden states. Note again (see Remark 3) that the assumption of a probabilistic relationship between hidden states and observed values, in the style of HMPs, does not generalize our treatment.*

The following statement is easy to verify.

Lemma 2. *Assume that the collection of k information functions X_1, \dots, X_k is jointly observable in the Markov state q , then every subcollection X_{i_1}, \dots, X_{i_m} is jointly observable in q . In particular, every individual information function X_i is observable. Moreover, if the X_i are real-valued, also every product $X_i X_j$ is observable in q .*

◇

Hence, if two information functions X and Y on the system \mathfrak{S} are real-valued and jointly observable, their product XY is statistically observable and has a well-defined expectation $E(XY)$.

Clearly, in our setting, any collection of information functions is jointly observable in any quantum density.

In the following two subsections, we will put our approach into context with earlier treatments.

6.1 Bell's inequality

The well-known inequality of Bell [4,5] takes the form from the following lemma in our context as a statement on the expectations of products of pairs of information functions.

Lemma 3 (Bell's inequality). *Let $X, Y, Z : \Omega \rightarrow \{-1, +1\}$ be arbitrary information functions on the system \mathfrak{S} , described by the density Q . If X, Y and Z are jointly observable relative to Q , then the following inequality holds:*

$$|E_Q(XY) - E_Q(YZ)| \leq 1 - E_Q(XZ) . \quad (67)$$

Proof. Any choice of $x, y, z \in \{-1, +1\}$ satisfies the inequality $|xy - yz| \leq 1 - xz$. Because of the joint observability assumption, all the observation probabilities

$$p_Q(x, y, z) = \Pr\{X = x, Y = y, Z = z\}$$

are nonnegative real numbers that sum up to 1. So we conclude

$$\begin{aligned} |E_Q(XY) - E_Q(YZ)| &= \left| \sum_{x,y,z} (xy - yz)p_Q(x, y, z) \right| \leq \sum_{x,y,z} |xy - yz|p_Q(x, y, z) \\ &\leq \sum_{x,y,z} (1 - xz)p_Q(x, y, z) = 1 - E_Q(XZ) . \end{aligned}$$

◇

Of course, Bell's inequality may be violated by information functions that are pairwise but not jointly observable, because triples, while not yet pairs of observables lead to identification of hidden states. We raise the following example. Consider a system \mathfrak{S} with a set $\Omega = \{\omega_1, \omega_2, \omega_3, \omega_4, \omega_5\}$ of five hidden states, for example, and three information functions $X, Y, Z : \Omega \rightarrow \{-1, +1\}$ as in the following table:

	ω_1	ω_2	ω_3	ω_4	ω_5	
X	-1	+1	-1	-1	-1	
Y	+1	+1	-1	+1	-1	
Z	+1	+1	+1	-1	-1	(68)

One can check that X, Y, Z are pairwise observable relative to the generalized density

$$Q = \text{diag}(-1/3, 1/3, 1/3, 1/3, 1/3) \quad (69)$$

and yield the product expectations

$$E_Q(XY) = +1, \quad E_Q(YZ) = -1/3, \quad E_Q(XZ) = +1 , \quad (70)$$

which violate Bell's inequality (67).

The explanation for this is that none of the value pairs from $\{-1, +1\} \times \{-1, +1\}$ is in a one-to-one correspondence with ω_1 , whose eigenvalue is negative, for any of the pairs $(X, Y), (X, Z), (Y, Z)$ as composite information functions. However, it holds that

$$(X, Y, Z)^{-1}(-1, +1, +1) = \{\omega_1\} \quad (71)$$

which puts ω_1 in a one-to-one correspondence with the value triple $(-1, +1, +1)$.

Remark 5 *Experimental results seem to indicate that quantum systems may violate Bell's inequality (see, e.g., Aspect et al. [2]). This is sometimes interpreted as showing that quantum mechanics does not admit a theory with hidden variables. The generalized density picture makes it clear that a violation of Bell's inequality only shows that the system is studied in terms of measurements that are perhaps pairwise but not jointly observable. The existence of definite but hidden states is not excluded. In fact, an experimentally observed violation of Bell's inequality suggests that one should not place a priori nonnegativity restrictions on concepts of states into which a system can be prepared.*

6.2 Feynman's approach to the EPR paradox

We raise another prominent example, originally put forward by Feynman [12]. This example served as an instance where the assumption of hidden states leads to contradictions. In this doing, Feynman was one of the first to provide a mathematical model to explain the Einstein, Rosen and Podolsky (EPR) paradox (see also Scully *et al.* [24]).

Feynman provides the example of a quantum density $Q \in \mathbb{C}^{2 \times 2}$ that reflects the preparation of a spin $1/2$ system, for spin along the $+x$ and $+z$ axis. Accordingly, he assumes the existence of 4 hidden states, which are in a one-to-one-correspondence with the value tuples $(++)$, $(+-)$, $(-+)$, $(--)$. According to the preparation (see [12,24] for details), relative frequencies, and in the limit, probabilities for those tuples can be realized by

$$\begin{aligned} P(++) &= [1 + \langle \hat{\sigma}_z \rangle + \langle \hat{\sigma}_x \rangle + \langle \hat{\sigma}_y \rangle]/4 \\ P(+-) &= [1 + \langle \hat{\sigma}_z \rangle - \langle \hat{\sigma}_x \rangle - \langle \hat{\sigma}_y \rangle]/4 \\ P(-+) &= [1 + \langle \hat{\sigma}_z \rangle + \langle \hat{\sigma}_x \rangle - \langle \hat{\sigma}_y \rangle]/4 \\ P(--) &= [1 - \langle \hat{\sigma}_z \rangle - \langle \hat{\sigma}_x \rangle - \langle \hat{\sigma}_y \rangle]/4, \end{aligned}$$

where $\langle \hat{\sigma}_x \rangle$, $\langle \hat{\sigma}_y \rangle$, $\langle \hat{\sigma}_z \rangle$ are the Pauli spin operators.

Feynman realized that, depending on the quantum density Q , some of these “probabilities” could be negative. For example, the situation

$$\langle \hat{\sigma}_x \rangle = \langle \hat{\sigma}_y \rangle = \langle \hat{\sigma}_z \rangle = 1/2, \quad (72)$$

which by choosing an appropriate (2×2) -dimensional Q is possible, yields $P(++) = 5/8$, $P(+-) = 1/8$, $P(-+) = 3/8$, $P(--) = -1/8$.

These values arise in the course of measurements, which are expressed by the Pauli operators. As measurements are supposed to yield statistically meaningful results—measuring value tuples relates to sampling one of $(++)$, ..., $(--)$, so the $P(++)$, ..., $P(--)$, as the limits of these sampling experiments, require statistical interpretation. So P not being a probability distribution leads to probabilistic conflicts. In order to resolve the issue, Feynman suggested to extend probability theory.

We do not have to do this. The concept of generalized densities leaves us with options Feynman did not have. In Feynman's example, eigenspaces immediately correspond to spin constellations. Our approach to Feynman's example, however, where

eigenspaces reflect hidden states, rather than other physical entities, starts from the generalized density

$$Q = \text{diag}(5/8, 1/8, 3/8, -1/8). \quad (73)$$

Here, the entries of Q , in particular $Q_{44} = -1/8$, are merely parameters that serve to describe the state of the system. Consequently, one does not need to interpret them further and one does not need to extend probability theory. We further provide

$$\begin{array}{c|cccc} & \omega_1 & \omega_2 & \omega_3 & \omega_4 \\ \hline X & + & + & - & - \\ Z & + & - & + & - \end{array} \quad (74)$$

as two information functions through which one has (potentially) observational access to values for the different spins. One realizes now that X and Z are not jointly measurable (observable). This means that there is no measuring device by which one can determine value pairs for X and Z simultaneously. However, by (58), it is easy to see that [again, let q_ω be the eigenvalue corresponding to hidden state ω]

$$\begin{aligned} (p_X)_Q(+) &= q_{\omega_1} + q_{\omega_2} = 3/4 \\ (p_X)_Q(-) &= q_{\omega_3} + q_{\omega_4} = 1/4 \end{aligned}$$

and, similarly, $(p_Y)_Q(+) = 1, (p_Y)_Q(-) = 0$, which points out that X and Z are measurable relative to Q .

The potential benefit of our approach is to formally integrate hidden states into system preparation. In Feynman's example, this is not possible. Hidden states can only come to life by the attempt to determine them via measurements. Those measurements involve to simultaneously perform two incompatible measurements [in terms of physics: note that the Pauli operators do not commute]. The assumption of the measurable existence of certain value tuples—the hidden states—resulting from two incompatible measurements leads to interpretational conflicts in Feynman's frame, but not in ours.

7 Conclusion

In this treatment, we have provided models that put quantum random walks, hidden Markov processes and finitary processes into a unifying context. The motivation for doing so was the earlier insight that not only hidden Markov processes, but also quantum random walks are finitary, which yielded efficient tests for equivalence and ergodicity also for quantum random walks. Since hidden states play a key role in these issues, our models provide a clear, formal access to such hidden states, now also in quantum random walks and their natural, quantum-style generalizations. The benefits of this are twofold: first, we have become able to re-visit hidden states in quantum mechanics also in the light of principles that apply for finitary processes (decoupling hidden states from probability theory), which can allow to (dramatically) reduce model complexity. Second, this line of research has pointed out how to obtain meaningful, quantum-style asymptotic properties for quantum random walks, and their generalizations. Last but

not least, our treatment helps to re-visit classical treatments on hidden states in quantum mechanics.

Future work of ours is to further explore the benefits of finitary processes in the context of quantum information theory. Since finitary processes both capture classical Markovian processes and quantum computing related Markovian-style processes, further unifying insights should be possible.

References

1. AHARONOV, D., AMBAINIS, A., KEMPE, J. and VAZIRANI, U. (2001). Quantum walks on graphs. *Proceedings of the 33th STOC*, ACM, New York, 60-69.
2. A. ASPECT, J. DALIBARD, G. ROGER: *Experimental tests of Bell's inequalities using time-varying analyzers*, Phys. Rev. Lett. 49, 1804 (1982).
3. O.E. BARNDORFF-NIELSEN, R.D. GILL, P.E. JUPP, *On quantum statistical inference*, J. Roy. Statist. Soc. B (2003), 775-816.
4. J.S. BELL: *On the Einstein Podolsky Rosen paradox*, Physics 1, 195-200 (1964).
5. J.S. BELL: *On the problem of hidden variables in quantum mechanics*, Rev. Mod. Phys. 38, 447-452 (1966).
6. BLACKWELL, D. and KOOPMANS, L. (1957). On the identifiability problem for functions of finite markov chains. *Annals of Mathematical Statistics* 28 1011-1015.
7. DHARMADHIKARI, S.W. (1965). A characterization of a class of functions of finite markov chains. *Annals of Mathematical Statistics* 36 524-528.
8. A. EINSTEIN, B. PODOLSKY, N. ROSEN: *Can quantum mechanical descriptions of physical reality be considered complete?*, Phys. Rev. 47, 777-780 (1935).
9. EPHRAIM, Y. and MERHAV, N. (2002). Hidden Markov Processes. *IEEE Transactions on Information Theory*, 48 1518-1569.
10. FAIGLE, U. and SCHOENHUTH, A. (2007). Asymptotic mean stationarity of sources with finite evolution dimension. *IEEE Transactions on Information Theory* 53(7) 2342-2348.
11. FAIGLE, U. and SCHÖNHUTH, A. (2011). Efficient tests for equivalence of hidden Markov processes and quantum random walks. *IEEE Transactions on Information Theory*, 57(3) 1746-1753.
12. R.P. FEYNMAN: *Quantum Implications, Essays in Honour of David Bohm*, B.J. Hiley and F.D. Peat eds., Routledge and Kegan Paul, London, 235-246 (1987).
13. FINESSO, L., GRASSI, A. and SPREIJ, P. (2010). Approximation of stationary processes by hidden Markov models. *Mathematics of Control, Signals and Systems* 22 1-22. Available at <http://arxiv.org/abs/math/0606591>.
14. GILBERT, E.J. (1959). On the identifiability problem for functions of finite Markov chains. *Annals of Mathematical Statistics* 30 688-697.
15. R.M. GRAY, *Probability, Random Processes, and Ergodic Properties*, Springer-Verlag, New York, 1988.
16. R.M. GRAY, *Entropy and Information Theory*, Springer-Verlag, New York, 1990.
17. HELLER, A. (1965). On stochastic processes derived from Markov chains. *Annals of Mathematical Statistics*, 36(4) 1286-1291.
18. ITO, H., AMARI, S.-I. and KOBAYASHI, K. (1992). Identifiability of hidden Markov information sources and their minimum degrees of freedom. *IEEE Transactions on Information Theory*, 38(2) 324-333.
19. JAEGER, H. (2000). Observable operator models for discrete stochastic time series. *Neural Computation* 12(6) 1371-1398.

20. J. KEMPE (2003). Quantum random walks: an introductory overview. *Contemporary Physics* **44**, 307-327.
21. W. MÜCKENHEIM, *A review of extended probabilities*, Physics Reports 133, 337-401 (1986).
22. W.M. DE MUYNCK AND OMAR ABU-ZEID, *On an alternative interpretation of the Bell inequalities*, Phys. Lett. 100A, 485-489 (1984).
23. M. NIELSEN AND I. CHUANG, *Quantum Computation and Quantum Information*, Cambridge University Press, 2000.
24. M.O. SCULLY, H. WALTHER AND W. SCHLEICH, *Feynman's approach to negative probability in quantum mechanics*, Phys. Rev. A 49, 1562-1566 (1994).
25. SCHÖNHUTH, A. and JAEGER, H. (2009). Characterization of ergodic hidden Markov sources. *IEEE Transactions on Information Theory*, **55(5)** 2107–2118.
26. SCHÖNHUTH, A. (2009). On analytic properties of entropy rate. *IEEE Transactions on Information Theory*, **55(5)** 2119–2127.
27. A. SCHÖNHUTH (2014). Generic identification of binary-valued hidden Markov processes, *Journal of Algebraic Statistics*, **5(1)**, 72-99.
28. M. SZEGEDY (2004). Quantum Speed-up of Markov Chain Based Algorithms, *Proceedings of the 45th FOCS*, IEEE, Rome, 32-41.
29. VIDYASAGAR, M. (2011). The complete realization problem for hidden Markov models: A survey and some new results. *Mathematics of Control, Signals and Systems*, **23(1)** 1–65.
30. M.M. WILDE, *From Classical to Quantum Shannon Theory*, arXiv:1106.1445 (2011).